

A parcel formulation for Hamiltonian layer models

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Starting from the three-dimensional hydrostatic primitive equations, we derive Hamiltonian N -layer models with isentropic tropospheric and isentropic or isothermal stratospheric layers. Our construction employs a new parcel Hamiltonian formulation which describes the fluid as a continuum of Hamiltonian ordinary differential equations bound together by integral transport laws. In particular, we show that this parcel Hamiltonian structure is compatible with the stacking of layers under isentropic or isothermal constraints. The appeal of the parcel formulation is the simplification of various calculations, in particular the derivation of the continuum Poisson bracket and the proof of the Jacobi identity. A comparison and connection is made between the Hamiltonian dynamics of fluid parcels and the Hamiltonian system of partial differential equations. The parcel formulation can be seen as a precursor and tool for the study of Hamiltonian numerical schemes.

1 Introduction

Compressible fluid mechanics has a well known Hamiltonian formulation in which all Eulerian fields—velocity, density, and potential temperature, if applicable—appear as variables in the associated Poisson structure (Shepherd 1990, Salmon 1998). This structure is generally destroyed under any kind of discretization. Less well known is the so-called parcel Hamiltonian formulation in which each infinitesimal fluid element evolves according to a non-autonomous Hamiltonian ordinary differential equation much akin to classical point-particle mechanics (Bokhove and Oliver 2006). Each single parcel Hamiltonian is the sum of its kinetic energy and an Eulerian potential evaluated at the parcel's position. Mass and energy transport remain, however, external to the Hamilton principle—they merely tie together the single parcel equations by providing non-autonomous contributions to the single parcel potentials. Thus, the parcel Hamiltonian formulation provides less structure than the classical continuum Hamiltonian formulation. Remarkably, the parcel formulation survives space-discretization by numerical particle methods, a fact which has been explored by Frank *et al.* (2002), and Frank and Reich (2003, 2004).

We remark that the parcel Hamiltonian formulation is formally weaker than the Hamiltonian formulation in Lagrangian coordinates, yet the former contains enough structure so that the latter can be systematically reconstructed. Part of the reconstruction involves mapping between the Poisson brackets in Eulerian and Lagrangian descriptions, which are well known (Morrison 1982, Holm *et al.* 1983, Marsden *et al.* 1984). The bracket associated with the parcel formulation can immediately be recognized as a localized version of the Poisson bracket in Lagrangian coordinates; this correspondence is trivially realized by choosing localized test functionals. However, the corresponding translation between the localized Hamilton *function* of the parcel formulation and the Hamilton *functional* of the Hamiltonian formulation in Lagrangian coordinates is more than a name change—it involves, in the forward direction, the equivalent of reconstruction of a potential from a gradient. We have previously studied this correspondence in the context of three (geophysical) fluid models: two-dimensional vortical systems in a generalized streamfunction-vorticity representation, the rotating shallow-water equations, and the three-dimensional compressible Euler equations for an ideal gas (Bokhove and Oliver 2006, Bokhove and Lynch 2007).

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The appeal of parcel formulations is two-fold. First, they provide a setting for the study and derivation of Hamiltonian particle methods that is more general than the smoothed particle hydrodynamic-type (SPH) schemes of Salmon (1983); in particular, Hamiltonian particle-mesh (HPM) methods as introduced by Frank *et al.* (2002) are included. It can be shown that any numerical scheme which preserves the parcel structure will have a circulation theorem in the sense of Frank and Reich (2003). Second, the derivation of the continuum Poisson brackets as well as the proof of the continuum Jacobi identity are greatly simplified by taking a parcel Poisson formulation as the starting point. The explicit computations behind the mapping of the Lagrangian to the Eulerian continuum Poisson bracket (Holm *et al.* 1983) are also easy to carry out using the parcel framework.

In this paper, we extend the discussion of parcel formulations to simplified models of the atmosphere that consist of N quasi-two-dimensional layers in each of which the flow is columnar. We demonstrate that, provided the layer flows satisfy a thermodynamic iso-constraint, the N -column Hamiltonian formulations (as we call the parcel Hamiltonian formulation when integrated over fluid columns) have matching conditions at the layer interfaces which are compatible with the structure. In particular, the layer Hamiltonians sum up to an N -layer Hamiltonian that can then be lifted to a full N -layer continuum Hamiltonian with easily computable N -layer Poisson bracket. While the latter is well known (Ripa 1993, Bokhove 2002), the derivation we offer is straightforward and new. Our primary motivation, however, lies in the parcel formulation as a precursor for HPM or Hamiltonian particle finite element discretizations of multilayer systems.

In the main body of the paper, we study the case of N isentropic layers. An isentropic model will be neutrally and statically stable provided the isentropes do not overturn and the values of the layer entropies increase upward. Here, the entropy is constant in each layer, so that, within each layer, only static stability is achieved. Yet, the stratification in the atmosphere, especially in the stratosphere, is typically strictly stable with strict monotonic increase of entropy with height (Birner 2006). Thus, isentropic layer models can be viewed as a piecewise constant approximation of hydrostatic gas dynamics with an increasing entropy profile. In other words, they constitute a finite volume approximation in the vertical.

In Appendix D, we show that a similarly layered column formulation can be achieved under isothermal conditions. On the one hand, this computation demonstrates how different iso-constraints lead to structurally similar Hamiltonian layered column systems. On the other hand, the observation that in the stratosphere temperature and buoyancy frequency are nearly constant (Birner *et al.* 2002), may give some limited physical motivation for studying isothermal conditions: It is conceivable that diabatic effects balance density variations following a fluid parcel such that temperature is nearly conserved on a fluid parcel, in contrast to the adiabatic basis of isentropic layer modeling. Note that depth variations in the velocity profile could be modeled by using multiple layers with the same temperature.

The paper is structured as follows. In Section 2, we introduce the parcel formulation of the hydrostatically balanced, inviscid and unforced primitive equations, which shall be the starting point for our construction. In Section 3 we restrict the dynamics to isentropic columnar motion and construct a stack of N such layers. In Section 4, we lift the column Poisson formulation to a full continuum Poisson formulation and derive the Eulerian equations of motion. The paper concludes with a short summary and discussion in Section 5. Two appendices present interesting variations of this theme. In Appendix C, we present an Eulerian-Lagrangian “in between” formulation of our system, and Appendix D introduces the isentropic-isothermal N -layer model.

2 Parcel equations of motion

The starting point of our derivation is the dynamics of a single parcel of an ideal gas in hydrostatic balance on the f -plane, located at position $\mathbf{X} = (\mathbf{X}_h, Z) = (X, Y, Z)$, with velocity $\mathbf{U} = (\mathbf{U}_h, W) = (U, V, W)$ and potential temperature Θ . Writing $\nabla_{\mathbf{U}_h} = (\partial/\partial U, \partial/\partial V)$ and $\nabla_{\mathbf{X}_h} = (\partial/\partial X, \partial/\partial Y)$ for derivatives with respect to the velocity and position coordinates, respectively, and setting $\mathbf{U}_h^\perp \equiv (-V, U)$ with corresponding notation for other vectorial quantities in the horizontal plane, we can state the parcel Eulerian-Lagrangian

equations of motion,

$$\frac{d\mathbf{X}_h}{dt} = \nabla_{\mathbf{U}_h} H_h = \mathbf{U}_h, \quad (1a)$$

$$\frac{d\mathbf{U}_h}{dt} = -f \nabla_{\mathbf{U}_h}^\perp H_h - \nabla_{\mathbf{X}_h} H_h = -f \mathbf{U}_h^\perp - \nabla_{\mathbf{X}_h} M, \quad (1b)$$

$$\frac{d\Theta}{dt} = 0, \quad (1c)$$

$$0 = -\frac{\partial M}{\partial Z}. \quad (1d)$$

The parcel energy is given by

$$H_h = H_h(\mathbf{X}, \mathbf{U}_h, \Theta, t) = \frac{1}{2} |\mathbf{U}_h|^2 + M(\mathbf{X}, \Theta, t), \quad (2)$$

where

$$M(\mathbf{X}, \Theta, t) = \Theta \Pi(\mathbf{X}, t) + gZ \quad \text{and} \quad \Pi(\mathbf{X}, t) = c_p \eta(\mathbf{X}, t)^\kappa \quad (3)$$

are the Montgomery potential and Exner function, respectively, expressed in terms of a dimensionless pressure $\eta(\mathbf{X}, t) = p(\mathbf{X}, t)/p_r$ with reference pressure p_r , and where $\kappa = R/c_p$ with R the gas constant and c_p the constant specific heat at constant pressure.

System (1) is the hydrostatic version of the parcel formulation of gas dynamics given in Bokhove and Oliver (2006). The vertical velocity W is absent in the parcel energy (2) because the small aspect ratio between vertical and horizontal length and velocity scales used in the hydrostatic approximation implies that $W^2 \ll |\mathbf{U}_h|^2$. In this formulation, the Montgomery potential is seen as an externally prescribed potential which is defined on the continuum so that, in particular, gradients can be taken. We stress that the Exner function has Eulerian arguments $\Pi = \Pi(\mathbf{x}, t)$ evaluated in (3) at the parcel's location $\mathbf{x} = \mathbf{X}$.

In principle, the parcel position $\mathbf{X}(t)$, velocity $\mathbf{U}(t)$, and potential temperature $\Theta(t)$ depend on the continuum of parcels and time. On the other hand, equations (1) and (2) provide a non-autonomous Hamiltonian formulation for a single fluid parcel characterized by the variables \mathbf{X}_h , \mathbf{U}_h , and Θ ; it is constrained because the hydrostatic approximation is made. In this picture, these variables are considered as functions of time with only parametric dependence on the particular Lagrangian label \mathbf{A} (Bokhove and Oliver 2006, Bokhove and Lynch 2007, Dixon and Reich 2004). We note that Θ plays formally the role of a (generalized) position coordinate; we could associate a trivial dual momentum variable to obtain a canonical Hamiltonian formulation. Consequently, the Montgomery potential (3) depends on 3+1 position variables which can be differentiated upon independently; the notation $\nabla_{\mathbf{X}}$ thus refers to the gradient with respect to the first three physical position coordinates.

Missing is therefore a continuity equation such that the pressure—through the equation of state—can be determined from densities and potential temperatures of all parcels. We thus define a flow map such that the Eulerian position of a fluid parcel with label \mathbf{a} is given by $\mathbf{x} = \boldsymbol{\chi}(\mathbf{a}, t)$ and the Eulerian velocity \mathbf{u} is implicitly defined by $\dot{\boldsymbol{\chi}}(\mathbf{a}, t) = \mathbf{u}(\boldsymbol{\chi}(\mathbf{a}, t), t)$. The position and velocity of the distinguished parcel with $\mathbf{a} = \mathbf{A}$ are then $\mathbf{X}(t) = \boldsymbol{\chi}(\mathbf{A}, t)$ and $\mathbf{U}(t) = \mathbf{u}(\boldsymbol{\chi}(\mathbf{A}, t), t)$. Finally, we introduce the Eulerian potential temperature $\theta(\mathbf{x}, t)$ by setting

$$\Theta \equiv \Theta(\mathbf{A}) = \theta(\boldsymbol{\chi}(\mathbf{A}, t), t) \quad (4)$$

(note that we are assuming adiabatic conditions—in general, Θ will be a function of time as well) and the Eulerian density via

$$\rho(\mathbf{x}, t) = \int \rho(\mathbf{a}, 0) \delta(\mathbf{x} - \boldsymbol{\chi}(\mathbf{a}, t)) \, d\mathbf{a} \quad (5)$$

with Dirac delta function $\delta(\cdot)$.

We will now show that system (1) coincides with the usual system of partial differential equations for the hydrostatic motion of an ideal gas. First, recall that the first law of thermodynamics for an ideal gas, with equation of state

$$p = \rho R T, \quad (6)$$

can be restated as

$$T ds = c_p dT - dp/\rho, \quad (7)$$

so that

$$\frac{T}{\theta} = \left(\frac{p}{p_r}\right)^\kappa = \eta^\kappa \quad \text{with} \quad \theta = T_r \exp\left(\frac{(s - s_r)}{c_p}\right), \quad (8)$$

where s is the parcel specific entropy, and s_r and T_r denote reference specific entropy and temperature, respectively (Gill, 1982). Eliminating T from (6) and (8), we obtain

$$\frac{p^{\kappa-1}}{p_r^\kappa} = \frac{1}{\rho R \theta}. \quad (9)$$

Since $\nabla_{\mathbf{X}}$ acts, by definition, only on the three classical position coordinates, it commutes with Θ . Hence, we take the derivative of the potential with respect to the Eulerian coordinates and evaluate it at the parcel's position, as for classical single-particle non-autonomous Hamiltonians (see, e.g., the introduction of Marsden and Ratiu 1994). Thus, using the relation of parcel to Eulerian potential temperature (4) and (9), we find

$$\nabla_{\mathbf{X}} M(\mathbf{X}(t), \Theta, t) = \Theta \nabla_{\mathbf{X}} \Pi(\mathbf{X}(t), t) + \nabla_{\mathbf{X}}(gZ) \quad (10a)$$

$$= \left[\theta(\mathbf{x}, t) \nabla \Pi(\mathbf{x}, t) + \nabla(gz) \right]_{\mathbf{x}=\mathbf{X}(t)} \quad (10b)$$

$$= \left[\frac{1}{\rho(\mathbf{x}, t)} \nabla p(\mathbf{x}, t) + \nabla(gz) \right]_{\mathbf{x}=\mathbf{X}(t)}. \quad (10c)$$

In particular, (10) implies that (1d) is equivalent to

$$0 = -\frac{1}{\rho} \frac{\partial p}{\partial z} - g. \quad (11)$$

We recognize the right hand side of (10) as terms in the usual PDE formulation, while the left hand side of (10) and, consequently, system (1) also make sense for a non-dense set of discrete parcel paths (though closure of a such a discrete system via the continuity relation certainly requires approximation). In this reading, (1) contains the horizontal trajectory equations, the horizontal hydrostatic momentum equations for one single fluid parcel for an ideal gas written in material form, hydrostatic balance, and conservation of potential temperature on a parcel. Since we can reconstruct the Eulerian pressure via (5) and (9), the entire fluid system is closed.

We close with four remarks. First, once we know the pressure, either through the closure relations (5) and (9) or from observation, we can calculate trajectories for *individual* fluid parcels in the non-autonomous Eulerian-Lagrangian formulation.

Second, an expression for the vertical velocity dZ/dt can, in principle, be derived by differentiation of the hydrostatic balance relation in time, thereby ensuring that the solution remains hydrostatic. However, an explicit expression for the vertical velocity is not required in what follows.

Third, the density is in fact the Jacobian

$$\frac{\partial \chi(\mathbf{a}, t)}{\partial \mathbf{a}} = \frac{\rho(\mathbf{a}, 0)}{\rho(\chi(\mathbf{a}, t), t)} \quad (12)$$

between fluid label \mathbf{a} and Eulerian coordinates $\mathbf{x} = \chi(\mathbf{a}, t)$. This relation is never explicitly required, but is implicitly contained in the derivation of (5) via

$$\rho(\mathbf{x}, t) = \int \rho(\mathbf{x}', t) \delta(\mathbf{x} - \mathbf{x}') d\mathbf{x}' = \int \rho(\mathbf{a}, 0) \delta(\mathbf{x} - \chi(\mathbf{a}, t)) d\mathbf{a}. \quad (13)$$

Similarly, we can write

$$\rho(\mathbf{x}, t) \theta(\mathbf{x}, t) = \int \rho(\mathbf{a}, 0) \Theta(\mathbf{a}) \delta(\mathbf{x} - \chi(\mathbf{a}, t)) d\mathbf{a}. \quad (14)$$

Mathematically, (13) can be interpreted as the push-forward of $\rho(\cdot, 0) d\mathbf{a}$ interpreted, for example, as a Radon measure by the flow map χ . Thus, (13) can be read, in slight abuse of notation, as

$$\int \phi(\mathbf{x}) \rho(\mathbf{x}, t) d\mathbf{x} = \int \phi(\chi(\mathbf{a}, t)) \rho(\mathbf{a}, 0) d\mathbf{a} \quad (15)$$

for all appropriately integrable test functions ϕ , with a corresponding expression for (14); see, for example, Appendix A in the paper of Cullen and Feldman (2006) on the semi-geostrophic equations. Here, however, we are not claiming an analytic framework for generalized solutions of hydrostatic compressible flow; for a review on rigorous results see, for example, Li and Wang (2008). Rather, our point is structural: the integral relations (13) and (14) can be used, formally, as a starting point to derive numerical particle methods upon discretizing the density as a finite linear combination of point masses while replacing the Dirac delta by a regularized shape function. Moreover, writing the mass transport law in the form (13) is convenient as it leads to formally correct manipulations. As an example, the Eulerian continuity equation emerges by taking the time derivative of (13), using (1) and the definition of the Eulerian velocity field \mathbf{u} via

$$\partial_t \rho(\mathbf{x}, t) = - \int \rho(\mathbf{a}, 0) \nabla \delta(\mathbf{x} - \chi(\mathbf{a}, t)) \cdot \mathbf{U}(\mathbf{a}, t) d\mathbf{a} \equiv - \nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)). \quad (16)$$

Again, a rigorous correspondence is beyond the scope of this paper but has been given, for example, in the landmark paper by DiPerna and Lions (1989).

Fourth, there is a way to derive the identity (10) by using only integral relations (13) and (14), without explicit reference to the Eulerian potential temperature defined in (4). This perspective is more satisfactory from a numerical viewpoint where discrete versions of these integral relations are the primary building blocks. We therefore start from a weak formulation, using an arbitrary test function $\rho(\mathbf{A}, 0) \Phi(\mathbf{A})$ —the extra $\rho(\mathbf{A}, 0)$ is unessential but simplifies the expressions visually—to find

$$\begin{aligned} \int \rho(\mathbf{a}, 0) \Phi(\mathbf{a}) \nabla_{\mathbf{x}} M(\Theta, \mathbf{X}, t) d\mathbf{a} &= \int \rho(\mathbf{a}, 0) \Phi(\mathbf{a}) (\Theta(\mathbf{a}) \nabla \Pi(\chi(\mathbf{a}, t), t) + g\mathbf{k}) d\mathbf{a} \\ &\stackrel{(14)}{=} \int \Phi(\chi^{-1}(\mathbf{x}, t)) \rho(\mathbf{x}, t) \theta(\mathbf{x}, t) \nabla \Pi(\mathbf{x}, t) d\mathbf{x} + \int \rho(\mathbf{a}, 0) \Phi(\mathbf{a}) g\mathbf{k} d\mathbf{a} \\ &\stackrel{(13)}{=} \int \rho(\mathbf{a}, 0) \Phi(\mathbf{a}) \left[\theta(\mathbf{x}, t) \nabla \Pi(\mathbf{x}, t) + g\mathbf{k} \right]_{\mathbf{x}=\chi(\mathbf{a}, t)} d\mathbf{a} \\ &= \int \rho(\mathbf{a}, 0) \Phi(\mathbf{a}) \left[\frac{1}{\rho(\mathbf{x}, t)} \nabla p(\mathbf{x}, t) + \nabla(gz) \right]_{\mathbf{x}=\chi(\mathbf{a}, t)} d\mathbf{a} \end{aligned} \quad (17)$$

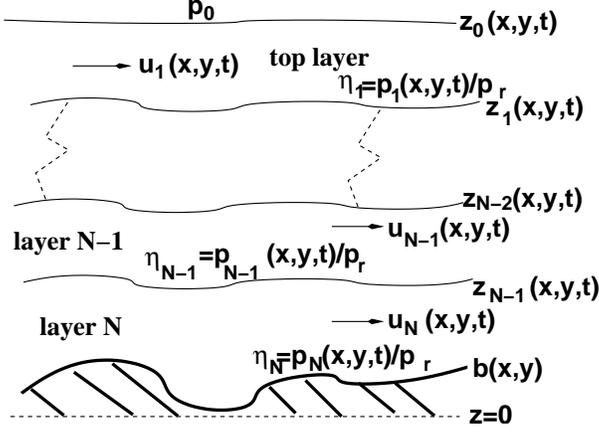


Figure 1. Sketch of the N -layer atmosphere. The interfaces $z = z_\alpha(\mathbf{x}, t)$ for $\alpha = 1, \dots, N - 1$ and the top of the upper stratospheric layer at $z = z_0(\mathbf{x}, t)$ are time dependent. The Earth's surface resides at $z = b(\mathbf{x}, t) = z_N(\mathbf{x}, t)$. Continuous and dimensionless pressures are defined at the interfaces and the Earth's surface using reference pressure p_r . The pressure $p_0 > 0$ at the top, $z = z_0(\mathbf{x}, t)$, is constant. Horizontal coordinates are $\mathbf{x}_h = (x, y)^T$ and time is denoted by t .

with \mathbf{k} the unit vector in the vertical. Note that $\mathbf{X} = \mathbf{X}(t) = \chi(\mathbf{A}, t)$. Since Φ is arbitrary, (10) follows again.

3 The N -layer isentropic model

In the following, we reduce the three-dimensional hydrostatic dynamics to a coupled system of N quasi-two-dimensional layers. To keep the N -layer model simple, we require that the parcels can be tied to a continuum by a continuity relation for a single scalar pseudo-density (to be introduced later). All thermodynamic potentials must be computable from parcel quantities and this pseudo-density, which amounts to constraining the thermodynamics to some isosurface. In this section, we exemplify the construction by assuming isentropic layers. Isothermal conditions can be treated much the same; the necessary changes are detailed in Appendix D.

The derivation proceeds in two steps. First, we derive the non-autonomous Hamiltonian parcel formulation for the isentropic N -layer model as a special case from the hydrostatic parcel model. Second, we show how to obtain a continuum formulation of this N -layer model by using continuity in an integral sense.

For each $\alpha = 1, \dots, N$, the layer labeled α ranges from $z_\alpha(\mathbf{x}_h, t) \leq z < z_{\alpha-1}(\mathbf{x}_h, t)$ at constant potential temperature θ_α ; see Fig. 1. We write $\eta_\alpha(\mathbf{x}_h, t) = p(\mathbf{x}_h, z_\alpha(\mathbf{x}_h, t), t)/p_r$ for $\alpha = 0, \dots, N$ to denote the dimensionless pressure at the interface between layer α and layer $\alpha + 1$. The bottom of the tropospheric layer $\alpha = N$ has prescribed stationary topography $z_N(\mathbf{x}_h, t) = b(\mathbf{x}_h)$ while the top layer surface at $z = z_0(\mathbf{x}_h, t)$ is free with fixed dimensionless pressure $\eta_0 > 0$, implying a positive temperature at z_0 through (8). To ensure neutral and static stability, we must require $\theta_{\alpha-1} > \theta_\alpha$.

In each isentropic layer, Eulerian potential temperature θ and parcel potential temperature Θ coincide, so that we can write the Montgomery potential directly in terms of θ and the dimensionless pressure $\eta(\mathbf{x}, t) = p(\mathbf{x}, t)/p_r$, *i.e.*

$$M = c_p \theta \eta^\kappa + g z. \quad (18)$$

Hydrostatic balance implies that M , within each layer, is independent of z ; see (11). Thus, (18) can be evaluated at any convenient height surface $z = z(\mathbf{x}_h, t)$.

At the Earth's surface, we can express the tropospheric Montgomery potential M_N in terms of the dimensionless surface pressure η_N and surface topography $b(\mathbf{x}_h)$,

$$M_N = c_p \theta_N \eta_N^\kappa + g b. \quad (19)$$

At the interface $z = z_\alpha$ between layer α and layer $\alpha + 1$ for $\alpha = 1, \dots, N - 1$, we have, due to continuity of the pressure and the z -independence of the Montgomery potentials,

$$M_\alpha = c_p \theta_\alpha \eta_\alpha^\kappa + g z_\alpha \quad (20)$$

and

$$M_{\alpha+1} = c_p \theta_{\alpha+1} \eta_\alpha^\kappa + g z_\alpha. \quad (21)$$

Rearranging, we obtain the recurrence relation

$$M_\alpha - M_{\alpha+1} = c_p (\theta_\alpha - \theta_{\alpha+1}) \eta_\alpha^\kappa \quad (22)$$

and therefore

$$M_\alpha = M_N + \sum_{\beta=\alpha}^{N-1} (M_\beta - M_{\beta+1}) = M_N + c_p \sum_{\beta=\alpha}^{N-1} (\theta_\beta - \theta_{\beta+1}) \eta_\beta^\kappa. \quad (23)$$

The free surface height z_0 may be recovered from the top layer Montgomery potential by noting that, at the free surface,

$$M_1 = c_p \theta_1 \eta_0^\kappa + g z_0. \quad (24)$$

Equating (24) with (23) for $\alpha = 1$ readily yields an expression for z_0 . When imposing rigid lid boundary conditions, it is actually more convenient to introduce an additional constant of integration $-(c_p \theta_1 \eta_0^\kappa + g Z_0)$ to the top layer Montgomery potential in (23), so that the top surface is characterized by $M_1 = 0$. It also may be reasonable to take $\eta_0 = 0$, implying zero temperature at the top of the atmosphere.

All N Montgomery potentials are seen to be Eulerian quantities and determined by the dimensionless Eulerian pressures $\eta_\alpha = \eta_\alpha(\mathbf{x}_h, t)$ for $\alpha = 1, \dots, N$ and topography $b = b(\mathbf{x}_h)$. Once they are known and evaluated at the location $\mathbf{x} = \mathbf{X}_\alpha$ of a layer's fluid parcel, the parcel trajectory can be calculated independent of all the other parcels. The coupling between the layers and between neighboring parcels within a layer is, again, prescribed in the form of a continuity equation. More specifically, we note that the mass of a slice of fluid of thickness dz in one of the layers with infinitesimal horizontal area $d\mathbf{x}_h$ is given, due to hydrostatic balance and with $\eta = p/p_r$, by

$$dm = \rho d\mathbf{x}_h dz = -d\mathbf{x}_h dp/g = -p_r d\mathbf{x}_h d\eta/g. \quad (25)$$

Integrating this relation across each layer, we obtain the mass of an infinitesimal fluid column within each layer with base area $d\mathbf{x}_h$ as the layer pseudo-densities

$$\sigma_\alpha = \int_{z_\alpha}^{z_{\alpha-1}} \rho dz = \frac{p_r}{g} \int_{\eta_{\alpha-1}}^{\eta_\alpha} d\eta = \frac{p_r}{g} (\eta_\alpha - \eta_{\alpha-1}), \quad (26)$$

where $\alpha = 1, \dots, N$. Incidentally, these relations explain our downward counting of the layers.

Note that our formulation allows the layer thickness to become zero. At these locations, the layer pseudo-density is also zero as the pressure drop cancels at the horizontal lines where σ_α vanishes. This happens, for example, for Earth-intersecting isentropes. Special boundary parcels demarcate the horizontal extent of an isentropic layer, both for fixed-wall boundaries and dynamic internal boundaries.

Let us now assume that the motion is columnar within each layer, *i.e.* that the initial velocities and, consequently, the velocities at any later time, are independent of z . We also, for simplicity, drop the layer index. Then, the flow map can be written as $\chi(\mathbf{a}, t) = (\chi_h(\mathbf{a}_h, t), \zeta(\mathbf{a}_h, c, t))$, where we now explicitly

distinguish the third component ζ of the three-dimensional parcel position $\boldsymbol{\chi}$ and the third label c of the three-dimensional label $\mathbf{a} = (\mathbf{a}_h, c)$, and its Jacobian decomposes multiplicatively (Miles and Salmon 1985). It is now easy to see that

$$\sigma(\mathbf{x}_h, t) = \int \sigma(\mathbf{a}_h, 0) \delta(\mathbf{x}_h - \boldsymbol{\chi}_h(\mathbf{a}_h, t)) \, d\mathbf{a}_h \quad (27)$$

with

$$\sigma(\mathbf{a}_h, 0) = \int_{z_{\text{bot}}(\mathbf{a}_h, 0)}^{z_{\text{top}}(\mathbf{a}_h, 0)} \rho(\mathbf{a}_h, c, 0) \, dc. \quad (28)$$

We are now ready to formulate a complete ‘‘column Hamiltonian formulation’’ of the continuum N -layer model. All vectors are now purely two-dimensional, so that we drop the subscript on horizontal vectors in the remainder of the paper. First, we have the hydrostatic parcel description (1), reduced to columnar motion, in each of the layers:

$$\frac{d\mathbf{X}_\alpha}{dt} = \nabla_{\mathbf{U}_\alpha} H_\alpha = \mathbf{U}_\alpha, \quad (29a)$$

$$\frac{d\mathbf{U}_\alpha}{dt} = -f \nabla_{\mathbf{U}_\alpha}^\perp H_\alpha - \nabla_{\mathbf{X}_\alpha} H_\alpha = -f \mathbf{U}_\alpha^\perp - \nabla_{\mathbf{X}_\alpha} M_\alpha \quad (29b)$$

with layer Hamiltonians

$$H_\alpha(\mathbf{X}_\alpha, \mathbf{U}_\alpha, t) = \frac{1}{2} |\mathbf{U}_\alpha|^2 + M_\alpha(\mathbf{X}_\alpha, t), \quad (29c)$$

where $\alpha = 1, \dots, N$. In this non-autonomous column Hamiltonian formulation, the four dependent variables are the horizontal column positions and velocities \mathbf{X}_α and \mathbf{U}_α . The layer Montgomery potentials are given by (19) and (23); they read

$$M_N(\mathbf{X}, t) = c_p \theta_N \eta_N(\mathbf{X}, t)^\kappa + g b(\mathbf{X}), \quad (29d)$$

$$M_\alpha(\mathbf{X}, t) = M_N(\mathbf{X}, t) + c_p \sum_{\beta=\alpha}^{N-1} (\theta_\beta - \theta_{\beta+1}) \eta_\beta(\mathbf{X}, t)^\kappa \quad (29e)$$

for $\alpha = 1, \dots, N-1$. The Montgomery potentials depend on the dimensionless pressures which, due to (26), can be written in terms of the pseudo-densities as

$$\eta_\alpha = \eta_0 + \frac{g}{p_r} \sum_{\beta=1}^{\alpha} \sigma_\beta \quad (29f)$$

for $\alpha = 1, \dots, N$.

Finally, the columns are tied together by the integral version of the continuity equation for the pseudo-densities,

$$\sigma_\alpha(\mathbf{x}, t) = \int \sigma_\alpha(\mathbf{a}, 0) \delta(\mathbf{x} - \boldsymbol{\chi}_\alpha(\mathbf{a}, t)) \, d\mathbf{a}. \quad (29g)$$

Let us summarize to re-emphasize the structure of the N -layer column model. Equations (29a–c) are, for each fixed label \mathbf{A} , a finite dimensional non-autonomous Hamiltonian system. We may write $\mathbf{X}_\alpha = \mathbf{X}_\alpha(t; \mathbf{A})$ and $\mathbf{U}_\alpha = \mathbf{U}_\alpha(t; \mathbf{A})$ to emphasize the parametric dependence of \mathbf{X}_α and \mathbf{U}_α on \mathbf{A} in the sense that the final

description, i.e. (29), does not involve derivatives with respect to \mathbf{A} . These systems form a continuum in the label space which is bound together by the integral continuity equation (29g) for the pseudo-densities σ_α . The pseudodensities feed back into the column Hamiltonian through the Montgomery potentials—this dependence renders the Hamiltonians time dependent.

System (29) is a closed form description of the fluid. It is different from the well-known Hamiltonian descriptions in terms of partial differential equations since the pseudodensities are external to the Hamiltonian structure. As such, it can be seen as a precursor to smoothed particle hydrodynamics (SPH) as derived variationally by Salmon (1983), Hamiltonian particle finite element methods, or Hamiltonian particle-mesh (HPM) methods like the ones described in Frank *et al.* (2002) and Frank and Reich (2004). These latter schemes differ from classical SPH since they involve Eulerian potentials and Eulerian discretizations thereof evaluated at the respective discrete particle positions (particles being the discretizations of the parcels such that discrete entities and continuum ones are clearly distinguished). As a consequence, the computations are in some instances faster, with symplectic time stepping guaranteeing phase-volume preservation.

In the next section, we show how to recover the well-known continuum Poisson structure from this new column Poisson structure.

4 Hamiltonian formulation

In this section we show how to write the N -layer column equations (29) in a *column Poisson formulation*, how to “lift” this column Poisson formulation to a partial differential (generalized) Poisson formulation, and, thereby, how to obtain the usual Eulerian description of the N -layer system. The derivation is relatively straightforward, but, to the best of our knowledge, has not appeared elsewhere.

We first note that (29a) and (29b) can be written as

$$\frac{dF}{dt} = \{F, H\}, \quad (30a)$$

where

$$\{F, G\} = \sum_{\alpha=1}^N \{F, G\}_\alpha = \sum_{\alpha=1}^N f \nabla_{\mathbf{U}_\alpha}^\perp F \cdot \nabla_{\mathbf{U}_\alpha} G + \nabla_{\mathbf{X}_\alpha} F \cdot \nabla_{\mathbf{U}_\alpha} G - \nabla_{\mathbf{X}_\alpha} G \cdot \nabla_{\mathbf{U}_\alpha} F \quad (30b)$$

for arbitrary functions F and G of \mathbf{X}_α , \mathbf{U}_α and t , and with Hamiltonian

$$H = \sum_{\alpha=1}^N H_\alpha = \sum_{\alpha=1}^N \frac{1}{2} |\mathbf{U}_\alpha|^2 + M_\alpha. \quad (30c)$$

The equations of motion (29a) and (29b) follow from (30) by taking $F = \mathbf{X}_\alpha$ and $F = \mathbf{U}_\alpha$, respectively. The bracket (30b) is skew-symmetric and satisfies the Jacobi identity

$$\{K, \{F, G\}\} + \{F, \{G, K\}\} + \{G, \{K, F\}\} = 0 \quad (31)$$

for arbitrary functions F, G and K as can be verified directly; it is canonical when $f = 0$. Note that the Hamiltonian H is not a constant of the motion as it depends, through the Montgomery potentials

$$M_\alpha = M_\alpha(\eta_\beta(\mathbf{X}_\alpha, t), b(\mathbf{X}_\alpha)), \quad (32)$$

functions of the scaled Eulerian pressures η , on time.

We will next derive a Hamiltonian formulation in the Eulerian variables $\mathbf{v}_\alpha = \mathbf{v}_\alpha(\mathbf{x}, t)$ and $\sigma_\alpha = \sigma_\alpha(\mathbf{x}, t)$ from the above column Poisson formulation. To do so, we need to relate the functional derivatives of arbitrary functionals \mathcal{F} and \mathcal{G} to partial derivatives for the functions F and G , and relate the time

derivative $d\mathcal{F}/dt$ of the functional \mathcal{F} to the time derivative dF/dt . From these relations and the column Hamiltonian formulation we then obtain a Poisson formulation

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\} \quad (33)$$

for the Eulerian Hamiltonian dynamics.

Evaluation of an Eulerian quantity such as the horizontal velocity $\mathbf{v}(\mathbf{x}, t)$ at the parcel position is denoted by $\dot{\chi} = \mathbf{v} \circ \chi$ which in the parcel picture is identified with the parcel (or column) velocity \mathbf{U} for the distinguished label \mathbf{A} . Mathematically, ‘ \circ ’ denotes the composition of maps; in the present context we can think of “ $(\cdot) \circ \chi(\mathbf{a}, t)$ ” signifying that an Eulerian variable (\cdot) is evaluated at the location $\mathbf{x} = \chi(\mathbf{a}, t)$ of the Lagrangian parcel \mathbf{a} . This notation is powerful because it allows a precise description denoting in which framework, Lagrangian or Eulerian, a variable is being considered. Using this notation, the relations between functional and function derivatives, and between the two brackets, are given by

$$\nabla_{\mathbf{U}_\alpha} F = \left(\frac{1}{\sigma_\alpha} \frac{\delta \mathcal{F}}{\delta \mathbf{v}_\alpha} \right) \circ \chi_\alpha(\mathbf{A}, t) \quad (34a)$$

$$\nabla_{\mathbf{x}_\alpha} F = \left(\nabla \frac{\delta \mathcal{F}}{\delta \sigma_\alpha} - \frac{1}{\sigma_\alpha} \frac{\delta \mathcal{F}}{\delta \mathbf{v}_\alpha} \cdot \nabla \mathbf{v}_\alpha \right) \circ \chi_\alpha(\mathbf{A}, t), \quad (34b)$$

and we have

$$\frac{d\mathcal{F}}{dt} = \int \frac{d}{dt} F \, d\mathbf{a} = \sum_{\alpha=1}^N \int \{F, H_\alpha\}_\alpha \, d\mathbf{a}, \quad (35)$$

see Appendix A for a proof. Substitution of (34) into (35) using (30b) yields the Hamiltonian dynamics of the N -layer equations (Shepherd 1990, in general; Ripa 1993 and Bokhove 2002, specifically) where, under the assumption that the horizontal boundary condition permits integration by parts with vanishing boundary contributions, we find

$$\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, \mathcal{H}\} = \sum_{\alpha=1}^N \int \left[q_\alpha \frac{\delta \mathcal{F}}{\delta \mathbf{v}_\alpha} \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{v}_\alpha} - \frac{\delta \mathcal{F}}{\delta \sigma_\alpha} \nabla \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{v}_\alpha} + \frac{\delta \mathcal{H}}{\delta \sigma_\alpha} \nabla \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{v}_\alpha} \right] d\mathbf{x} \quad (36)$$

with Hamiltonian

$$\mathcal{H} = \sum_{\alpha=1}^N \int \sigma_\alpha \left(\frac{1}{2} |\mathbf{v}_\alpha|^2 + g b \right) d\mathbf{x} + \frac{p_r c_p}{g(\kappa + 1)} \int \left(\sum_{\alpha=1}^{N-1} (\theta_\alpha - \theta_{\alpha+1}) \eta_\alpha^{\kappa+1} + \theta_N \eta_N^{\kappa+1} \right) d\mathbf{x} \quad (37)$$

and layer potential vorticity

$$q_\alpha = (f + \nabla^\perp \cdot \mathbf{v}_\alpha) / \sigma_\alpha. \quad (38)$$

The potential vorticity is computed explicitly in Appendix A. The Hamiltonian is required to satisfy (A.13) and (A.15) for each layer, namely

$$\frac{\delta \mathcal{H}}{\delta \mathbf{v}_\alpha} = \sigma_\alpha \mathbf{v}_\alpha, \quad (39a)$$

$$\frac{\delta \mathcal{H}}{\delta \sigma_\alpha} = \frac{1}{2} |\mathbf{v}_\alpha|^2 + M_\alpha. \quad (39b)$$

These conditions are consistent with our previously derived expressions for the Montgomery potentials (29d) and (29e) due to the relationship between the (scaled) pressures and pseudo-densities given by (29f), which implies that

$$\frac{\partial \eta_\beta}{\partial \sigma_\alpha} = \begin{cases} g/p_r & \text{if } \alpha \leq \beta \\ 0 & \text{if } \alpha > \beta, \end{cases} \quad (40)$$

so that

$$\frac{\delta \mathcal{H}}{\delta \sigma_\alpha} = \sum_{\beta=1}^N \frac{\delta \mathcal{H}}{\delta \eta_\beta} \frac{\partial \eta_\beta}{\partial \sigma_\alpha} = \frac{g}{p_r} \sum_{\beta=\alpha}^N \frac{\delta \mathcal{H}}{\delta \eta_\beta}. \quad (41)$$

When isentropes intersect the Earth, the horizontal extent of the affected layer becomes dynamic. It is given by the region where $\sigma_\alpha > 0$. No extra variations are required as $\sigma_\alpha = 0$ at the dynamic boundary of the Earth-intersecting isentrope. This situation is akin to the dynamic water-line movement in the shallow water equations, where the depth is zero at the water line.

The bracket (36) is skew-symmetric, which follows by inspection, and satisfies the Jacobi identity

$$\{\mathcal{F}, \{\mathcal{G}, \mathcal{K}\}\} + \{\mathcal{G}, \{\mathcal{K}, \mathcal{F}\}\} + \{\mathcal{K}, \{\mathcal{F}, \mathcal{G}\}\} = 0, \quad (42)$$

see Appendix B for a proof.

Finally, by inserting the test functionals

$$\mathcal{F} = \sigma_\alpha(\mathbf{x}, t) = \int \sigma_\alpha(\mathbf{x}', t) \delta(\mathbf{x} - \mathbf{x}') d\mathbf{x}' \quad (43)$$

and

$$\mathcal{F} = \mathbf{v}_\alpha(\mathbf{x}, t) = \int \mathbf{v}_\alpha(\mathbf{x}', t) \delta(\mathbf{x} - \mathbf{x}') d\mathbf{x}', \quad (44)$$

respectively, into (36), we obtain the Eulerian equations of motion

$$\frac{\partial \sigma_\alpha}{\partial t} = -\nabla \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{v}_\alpha} = -\nabla \cdot (\sigma_\alpha \mathbf{v}_\alpha), \quad (45a)$$

$$\frac{\partial \mathbf{v}_\alpha}{\partial t} = -q_\alpha \frac{\delta \mathcal{H}}{\delta \mathbf{v}_\alpha}^\perp - \nabla \frac{\delta \mathcal{H}}{\delta \sigma_\alpha} = -q_\alpha \sigma_\alpha \mathbf{v}_\alpha^\perp - \nabla \left(\frac{1}{2} |\mathbf{v}_\alpha|^2 + M_\alpha \right). \quad (45b)$$

This concludes the derivation of the N -layer isentropic atmospheric model and its Hamiltonian formulation. Owing to this Hamiltonian formulation, the model has conservation laws for energy, mass, and also local and global potential vorticity invariants (see, e.g., Salmon 1998).

5 Summary and conclusion

A layer model with N isentropic layers was derived using Hamiltonian methods in two ways. First, we simplified a parcel formulation of the hydrostatically-balanced primitive equations to Hamiltonian fluid parcel dynamics in N isentropic layers. Second, we connected this parcel formulation to the classical Eulerian Hamiltonian partial differential equations of motion for the N -layer model. While the former, parcel formulation consisted of ordinary differential equations for each fluid parcel and an integral relation gluing all parcels to a continuum, the latter, classical formulation is expressed entirely in terms of partial differential equations. We showed how these two formulations are connected. Both Hamiltonian formulations can be

used to explore the stability of geophysical flows and asymptotic models, using the associated conservation laws. Moreover, Hamiltonian parcel representations are continuum analogs of numerical Hamiltonian particle methods such as those devised by Frank *et al.* (2002), and Frank and Reich (2003, 2004) which preserve the parcel Hamiltonian structure with corresponding discrete conservation laws. Given the parcel formulations developed here, these layerwise stratified models can be developed directly into Hamiltonian particle methods or Hamiltonian particle finite element models. The key observation is that particle advection naturally preserves the parcel bracket. The overall scheme is energy-conserving provided one can design a suitable discretization of the potential; see, e.g., Frank and Reich (2003) and Dixon and Reich (2004).

The measured vertical temperature profiles shown by Birner *et al.* (2002) and Birner (2006) reveal that the temperature is nearly constant in at least a stratospheric layer ranging from roughly 10 to 20 km. These observations suggest that an isothermal layer model has some validity in the stratosphere. Such a model warrants two remarks. First, the observed velocity profile is depth dependent. This can be accommodated by taking multiple isothermal layers of the same temperature but with piecewise constant velocity profiles. Second, the diabatic effects ensuring the temperature to be constant in the observations emerge likely on a slower time scale than the one for the dynamics. For slow balanced vortical dynamics in the stratosphere this difference in time scale is then less extreme. In Appendix D, we have therefore constructed a N -layer model with isentropic tropospheric layers and isothermal stratospheric layers. We stress that our main intent is not the claim of applicability, but rather to give another exposition of the techniques used in the main text.

A future aim is to compare conservative numerical layer models based on either the parcel formulation or the partial differential one. Simulations with mixed isentropic and isothermal layers will form an interesting test case with potential for comparison with measured atmospheric temperature profiles.

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Appendix A

Derivation of the generalized Poisson bracket

We seek to associate to each column function $F = F(\mathbf{U}_1, \mathbf{X}_1, \dots, \mathbf{U}_N, \mathbf{X}_N)$ an Eulerian column functional $\mathcal{F} = \mathcal{F}[\mathbf{v}_1, \sigma_1, \dots, \mathbf{v}_N, \sigma_N]$. To this end, we must relate the partial derivatives of F to the variational derivatives of \mathcal{F} .

The computations can be done layer-wise, so that, for clarity of notation, we omit the layer indices. The general case follows by summation over layers. First, we write $\delta\boldsymbol{\chi}$ to denote the variation of $\boldsymbol{\chi}$ and define an Eulerian variation vector field \mathbf{w} via $\delta\boldsymbol{\chi} = \mathbf{w} \circ \boldsymbol{\chi}$ or, equivalently, $\mathbf{w} = \delta\boldsymbol{\chi} \circ \boldsymbol{\chi}^{-1}$, where the inverse flow map $\boldsymbol{\chi}^{-1}$ maps coordinate to label space. In other words, $\mathbf{w} = \mathbf{w}(\mathbf{x}, t)$ is the Eulerian representation of $\delta\boldsymbol{\chi}$. Then the following identities are true:

$$\delta\mathbf{v} \circ \boldsymbol{\chi} = \delta\dot{\boldsymbol{\chi}} - \nabla\mathbf{v} \circ \boldsymbol{\chi} \delta\boldsymbol{\chi}, \quad (\text{A.1})$$

$$\delta\sigma + \nabla \cdot (\mathbf{w}\sigma) = 0. \quad (\text{A.2})$$

The first identity follows directly by taking the variational derivative of $\dot{\boldsymbol{\chi}} = \mathbf{v} \circ \boldsymbol{\chi}$. The second identity can be seen as a continuity equation with respect to the variation vector field \mathbf{w} , and is shown as follows. Use

expression (29g) for σ , take the variational derivative and apply the result to an arbitrary test function ϕ . Then, using the chain rule and integration by parts, we have

$$\begin{aligned}
\int \phi \delta\sigma \, d\mathbf{x} &= - \int \phi(\mathbf{x}) \int \sigma(\mathbf{a}, 0) \nabla \delta(\mathbf{x} - \boldsymbol{\chi}(\mathbf{a})) \cdot \delta\boldsymbol{\chi} \, d\mathbf{a} \, d\mathbf{x} \\
&= \int \nabla \phi(\mathbf{x}) \cdot \int \sigma(\mathbf{a}, 0) \delta(\mathbf{x} - \boldsymbol{\chi}(\mathbf{a})) \delta\boldsymbol{\chi} \, d\mathbf{a} \, d\mathbf{x} \\
&= \int \nabla \phi(\mathbf{x}) \cdot \int \sigma(\mathbf{x}', t) \delta(\mathbf{x} - \mathbf{x}') \mathbf{w}(\mathbf{x}') \, d\mathbf{x}' \, d\mathbf{x} \\
&= - \int \phi(\mathbf{x}) \nabla \cdot (\mathbf{w}\sigma) \, d\mathbf{x}.
\end{aligned} \tag{A.3}$$

We first compute, on the continuum level,

$$\begin{aligned}
\delta\mathcal{F} &= \int \left[\frac{\delta\mathcal{F}}{\delta\mathbf{v}} \cdot \delta\mathbf{v} + \frac{\delta\mathcal{F}}{\delta\sigma} \delta\sigma \right] d\mathbf{x} \\
&= \int \left(\frac{1}{\sigma} \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi} \cdot (\delta\dot{\boldsymbol{\chi}} - \nabla\mathbf{v} \circ \boldsymbol{\chi} \delta\boldsymbol{\chi}) \, d\mathbf{a} - \int \frac{\delta\mathcal{F}}{\delta\sigma} \nabla \cdot (\mathbf{w}\sigma) \, d\mathbf{x} \\
&= \int \left(\frac{1}{\sigma} \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi} \cdot \delta\dot{\boldsymbol{\chi}} \, d\mathbf{a} + \int \left(\nabla \frac{\delta\mathcal{F}}{\delta\sigma} - \frac{1}{\sigma} (\nabla\mathbf{v})^T \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi} \cdot \delta\boldsymbol{\chi} \, d\mathbf{a}.
\end{aligned} \tag{A.4}$$

We now restrict our variations to a single column \mathbf{A} by assuming the special form

$$\delta\dot{\boldsymbol{\chi}}(\mathbf{a}, t) = \delta(\mathbf{a} - \mathbf{A}) \delta\mathbf{U}(t), \quad \delta\boldsymbol{\chi}(\mathbf{a}, t) = \delta(\mathbf{a} - \mathbf{A}) \delta\mathbf{X}(t), \tag{A.5}$$

so that

$$\delta\mathcal{F}(\mathbf{A}) = \left(\frac{1}{\sigma} \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi}(\mathbf{A}) \cdot \delta\mathbf{U} + \left(\nabla \frac{\delta\mathcal{F}}{\delta\sigma} - \frac{1}{\sigma} (\nabla\mathbf{v})^T \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi}(\mathbf{A}) \cdot \delta\mathbf{X}. \tag{A.6}$$

On the other hand, we have

$$\delta F = \frac{\partial F}{\partial \mathbf{U}} \cdot \delta\mathbf{U} + \frac{\partial F}{\partial \mathbf{X}} \cdot \delta\mathbf{X}, \tag{A.7}$$

whence, identifying $\delta\mathcal{F}(\mathbf{A}) = \delta F(\mathbf{U}, \mathbf{X})$ and comparing coefficients, we find that

$$\left(\frac{1}{\sigma} \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi}(\mathbf{A}) = \frac{\partial F}{\partial \mathbf{U}}, \tag{A.8a}$$

$$\left(\nabla \frac{\delta\mathcal{F}}{\delta\sigma} - \frac{1}{\sigma} (\nabla\mathbf{v})^T \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi}(\mathbf{A}) = \frac{\partial F}{\partial \mathbf{X}}. \tag{A.8b}$$

Next, note that all of the above computation up to (A.4) holds when the variational derivative is replaced

by a time derivative and, correspondingly, \mathbf{w} is replaced by \mathbf{v} . We find that

$$\begin{aligned}
\frac{d\mathcal{F}}{dt} &= \int \left(\frac{1}{\sigma} \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi} \cdot \ddot{\boldsymbol{\chi}} \, da + \int \left(\nabla \frac{\delta\mathcal{F}}{\delta\sigma} - \frac{1}{\sigma} (\nabla\mathbf{v})^T \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi} \cdot \dot{\boldsymbol{\chi}} \, da \\
&= \int \left[\frac{\partial F}{\partial \mathbf{U}} \cdot \ddot{\boldsymbol{\chi}} + \frac{\partial F}{\partial \mathbf{X}} \cdot \dot{\boldsymbol{\chi}} \right] da \\
&= \int \frac{d}{dt} F(\mathbf{U}, \mathbf{X}) \, da = \int \{F, H\} \, da,
\end{aligned} \tag{A.9}$$

where, in the second equality, we have inserted relations (A.8). We identify the last integral as the continuum Poisson bracket, which we can write in terms of functional derivatives as

$$\begin{aligned}
\{\mathcal{F}, \mathcal{G}\} &\equiv \int \{F, G\} \, da = \int \left[f \nabla_{\mathbf{U}}^{\perp} F \cdot \nabla_{\mathbf{U}} G + \nabla_{\mathbf{X}} F \cdot \nabla_{\mathbf{U}} G - \nabla_{\mathbf{X}} G \cdot \nabla_{\mathbf{U}} F \right] da \\
&= \int \left[\frac{f}{\sigma^2} \frac{\delta\mathcal{F}^{\perp}}{\delta\mathbf{v}} \cdot \frac{\delta\mathcal{G}}{\delta\mathbf{v}} + \left(\nabla \frac{\delta\mathcal{F}}{\delta\sigma} - \frac{1}{\sigma} (\nabla\mathbf{v})^T \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right) \cdot \frac{1}{\sigma} \frac{\delta\mathcal{G}}{\delta\mathbf{v}} \right. \\
&\quad \left. - \frac{1}{\sigma} \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \cdot \left(\nabla \frac{\delta\mathcal{G}}{\delta\sigma} - \frac{1}{\sigma} (\nabla\mathbf{v})^T \frac{\delta\mathcal{G}}{\delta\mathbf{v}} \right) \right] \circ \boldsymbol{\chi} \, da \\
&= \int \left[q \frac{\delta\mathcal{F}^{\perp}}{\delta\mathbf{v}} \cdot \frac{\delta\mathcal{G}}{\delta\mathbf{v}} + \nabla \frac{\delta\mathcal{F}}{\delta\sigma} \cdot \frac{\delta\mathcal{G}}{\delta\mathbf{v}} - \nabla \frac{\delta\mathcal{G}}{\delta\sigma} \cdot \frac{\delta\mathcal{F}}{\delta\mathbf{v}} \right] dx
\end{aligned} \tag{A.10}$$

with layer potential vorticity

$$q = \frac{f + \nabla^{\perp} \cdot \mathbf{v}}{\sigma}. \tag{A.11}$$

Hence, we have found (36) in the main text, but for an integration by parts.

Finally, we use (A.8) to derive the Hamiltonian functional \mathcal{H} . From (A.8a),

$$\left(\frac{1}{\sigma} \frac{\delta\mathcal{H}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi}(\mathbf{A}) = \frac{\partial H}{\partial \mathbf{U}} = \mathbf{U}, \tag{A.12}$$

so that

$$\frac{\delta\mathcal{H}}{\delta\mathbf{v}} = \sigma\mathbf{v}. \tag{A.13}$$

Further, from (A.8b),

$$\left(\nabla \frac{\delta\mathcal{H}}{\delta\sigma} - \frac{1}{\sigma} (\nabla\mathbf{v})^T \frac{\delta\mathcal{H}}{\delta\mathbf{v}} \right) \circ \boldsymbol{\chi}(\mathbf{A}) = \frac{\partial H}{\partial \mathbf{X}} = \nabla M, \tag{A.14}$$

so that, up to a constant of integration,

$$\frac{\delta\mathcal{H}}{\delta\sigma} = \frac{1}{2} |\mathbf{v}|^2 + M. \tag{A.15}$$

Appendix B

It is easy to check, by taking the total variation and localizing to a single column as in (A.5), that (A.8) hold in particular for functional-function pairs

$$\mathcal{J} = \int J(\dot{\boldsymbol{\chi}}, \boldsymbol{\chi}) \, \mathrm{d}\mathbf{a} \quad (\text{B.1})$$

with functional \mathcal{J} and function J . In particular, due to the first identity in (A.10), these relations hold when

$$\mathcal{J} = \{\mathcal{G}, \mathcal{K}\} \equiv \int \{G, K\} \, \mathrm{d}\mathbf{a}, \quad (\text{B.2})$$

so that, using (A.10) once more,

$$\{\mathcal{F}, \{\mathcal{G}, \mathcal{K}\}\} = \int \{F, \{G, K\}\} \, \mathrm{d}\mathbf{a}. \quad (\text{B.3})$$

Since the function bracket (30b) in integral (B.3), for each layer, satisfies the Jacobi identity by direct verification, the Jacobi identity (42) for the functional bracket is immediate.

Appendix C

Generalized Eulerian–Lagrangian Poisson formulation

In the body of this paper, we showed how to “lift” a column Poisson formulation to a generalized partial differential Poisson formulation which is equivalent to the usual Eulerian fluid description. Here, we show that it is also possible to derive a Poisson formulation which retains the Lagrangian description of the velocity, but incorporates the Eulerian pseudo-densities into the bracket. We can think of this formulation as being half-way between our column Poisson formulation where densities are external to the Hamiltonian structure and the fully Eulerian generalized Poisson formulation of Section 4. While the end result will not come as a surprise, we believe that the structure exposed in the derivation may be useful for the derivation of Hamiltonian numerical schemes.

In this Eulerian–Lagrangian formulation, we take $\mathbf{v}_\alpha^L = \mathbf{v}_\alpha(\boldsymbol{\chi}(\mathbf{a}, t), t)$ and $\sigma_\alpha = \sigma_\alpha(\mathbf{x}, t)$ as dependent variables. Then, the analog of (A.4) for a column functional $\mathcal{F} = \mathcal{F}[\mathbf{v}_1^L, \sigma_1, \dots, \mathbf{v}_N^L, \sigma_N]$ reads

$$\delta\mathcal{F} = \int \frac{\delta\mathcal{F}}{\delta\mathbf{v}^L} \cdot \delta\mathbf{v}^L \, \mathrm{d}\mathbf{a} + \int \frac{\delta\mathcal{F}}{\delta\sigma} \delta\sigma \, \mathrm{d}\mathbf{x} = \int \frac{\delta\mathcal{F}}{\delta\mathbf{v}^L} \cdot \delta\dot{\boldsymbol{\chi}}(\mathbf{a}) \, \mathrm{d}\mathbf{a} + \int \left(\nabla \frac{\delta\mathcal{F}}{\delta\sigma} \right) \circ \boldsymbol{\chi}(\mathbf{a}) \cdot \delta\boldsymbol{\chi}(\mathbf{a}) \, \mathrm{d}\mathbf{a}, \quad (\text{C.1})$$

where, as before, we are omitting column indices. Again, we restrict our variations to a single column \mathbf{A} by assuming the special form (A.5), so that

$$\delta\mathcal{F}(\mathbf{A}) = \frac{\delta\mathcal{F}}{\delta\mathbf{v}^L}(\mathbf{A}) \cdot \delta\mathbf{U} + \left(\nabla \frac{\delta\mathcal{F}}{\delta\sigma} \right) \circ \boldsymbol{\chi}(\mathbf{A}) \cdot \delta\mathbf{X}. \quad (\text{C.2})$$

On the other hand, we have (A.7), whence, identifying $\delta\mathcal{F}(\mathbf{A}) = \delta F(\mathbf{U}, \mathbf{X})$ and comparing coefficients, we

find that

$$\frac{\delta \mathcal{F}}{\delta \mathbf{v}^L}(\mathbf{A}) = \frac{\partial F}{\partial \mathbf{U}}, \quad (\text{C.3a})$$

$$\left(\nabla \frac{\delta \mathcal{F}}{\delta \sigma} \right) \circ \chi(\mathbf{A}) = \frac{\partial F}{\partial \mathbf{X}}. \quad (\text{C.3b})$$

Consequently, (A.9) must be replaced by

$$\frac{d\mathcal{F}}{dt} = \int \frac{\delta \mathcal{F}}{\delta \mathbf{v}^L} \cdot \dot{\chi} \, d\mathbf{a} + \int \left(\nabla \frac{\delta \mathcal{F}}{\delta \sigma} \right) \circ \chi \cdot \dot{\chi} \, d\mathbf{a} = \int \frac{d}{dt} F(\mathbf{U}, \mathbf{X}) \, d\mathbf{a} = \int \{F, H\} \, d\mathbf{a}, \quad (\text{C.4})$$

We identify the last integral as the continuum Poisson bracket, which we can write in terms of functional derivatives as

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\} &= \int \left[f \nabla_{\mathbf{U}}^{\perp} F \cdot \nabla_{\mathbf{U}} G + \nabla_{\mathbf{X}} F \cdot \nabla_{\mathbf{U}} G - \nabla_{\mathbf{X}} G \cdot \nabla_{\mathbf{U}} F \right] d\mathbf{a} \\ &= \int \left[f \frac{\delta \mathcal{F}}{\delta \mathbf{v}^L} \cdot \frac{\delta \mathcal{G}}{\delta \mathbf{v}^L} + \left(\nabla \frac{\delta \mathcal{F}}{\delta \sigma} \right) \circ \chi \cdot \frac{\delta \mathcal{G}}{\delta \mathbf{v}^L} - \left(\nabla \frac{\delta \mathcal{G}}{\delta \sigma} \right) \circ \chi \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{v}^L} \right] d\mathbf{a}. \end{aligned} \quad (\text{C.5})$$

To derive the corresponding Hamiltonian functional, note that, from (C.3a),

$$\frac{\delta \mathcal{H}}{\delta \mathbf{v}^L(\mathbf{A}, t)} = \frac{\partial H}{\partial \mathbf{U}} = \mathbf{U}, \quad (\text{C.6})$$

so that

$$\frac{\delta \mathcal{H}}{\delta \mathbf{v}^L} = \mathbf{v}^L. \quad (\text{C.7})$$

Further, from (C.3b),

$$\left(\nabla \frac{\delta \mathcal{H}}{\delta \sigma} \right) \circ \chi(\mathbf{A}) = \frac{\partial H}{\partial \mathbf{X}} = \nabla M, \quad (\text{C.8})$$

so that, up to a constant of integration,

$$\frac{\delta \mathcal{H}}{\delta \sigma} = M. \quad (\text{C.9})$$

By combining (C.7) and (C.9) for all N layers using the expression for the Montgomery potentials (29d) and (29e), we obtain the Hamiltonian functional

$$\mathcal{H} = \sum_{\alpha=1}^N \int \frac{1}{2} |\mathbf{v}_{\alpha}^L|^2 \, d\mathbf{a} + \sum_{\alpha=1}^N \int g \sigma_{\alpha} b \, d\mathbf{x} + \frac{p_r c_p}{g(\kappa+1)} \int \left(\sum_{\alpha=1}^{N-1} (\theta_{\alpha} - \theta_{\alpha+1}) \eta_{\alpha}^{\kappa+1} + \theta_N \eta_N^{\kappa+1} \right) d\mathbf{x} \quad (\text{C.10})$$

By substituting the test functionals

$$\mathcal{F} = \sigma_{\alpha}(\mathbf{x}, t) = \int \sigma_{\alpha}(\mathbf{x}', t) \delta(\mathbf{x} - \mathbf{x}') \, d\mathbf{x}' \quad (\text{C.11})$$

and

$$\mathcal{F} = \mathbf{v}_\alpha^L(\mathbf{a}, t) = \int \mathbf{v}_\alpha^L(\mathbf{A}, t) \delta(\mathbf{a} - \mathbf{A}) \, d\mathbf{a}, \quad (\text{C.12})$$

respectively, into (C.4) and (C.5), we obtain the mixed Eulerian–Lagrangian equations of motion

$$\frac{\partial \sigma_\alpha}{\partial t} = -\nabla \cdot \left(\sigma_\alpha \frac{\delta \mathcal{H}}{\delta \mathbf{v}_\alpha^L} \circ \chi^{-1} \right) = -\nabla \cdot (\sigma_\alpha \mathbf{v}_\alpha), \quad (\text{C.13a})$$

$$\frac{\partial \mathbf{v}_\alpha^L}{\partial t} = -f \frac{\delta \mathcal{H}}{\delta \mathbf{v}_\alpha^L}^\perp - \left(\nabla \frac{\delta \mathcal{H}}{\delta \sigma_\alpha} \right) \circ \chi(\mathbf{A}) = -f \mathbf{v}_\alpha^{L\perp} - (\nabla M_\alpha) \circ \chi(\mathbf{A}). \quad (\text{C.13b})$$

Appendix D

Model with isentropic tropospheric layers and isothermal stratospheric layers

Our method for deriving generalized partial differential Poisson formulations is not restricted to only isentropic layers. Physically relevant and interesting are models where the troposphere consists of multiple isentropic and the stratosphere of multiple isothermal layers, although from a mathematical point of view we can have arbitrary sequences of iso-layers.

To be consistent, isothermal models require that we give up material conservation of potential temperature (assuming that the iso-condition is maintained by external heat fluxes or dissipation), and that temperature is a materially conserved quantity as well.

Isentropic layers are used in the troposphere, as in Section 3. Likewise, in an isothermal layer $T = \theta \eta^\kappa$ is constant. The ideal gas law $p = \rho RT$ and hydrostatic balance $d \ln \eta / dz = -g / (RT)$ then imply that the buoyancy frequency satisfies

$$N^2 \equiv g \frac{d \ln \theta}{dz} = \frac{\kappa g^2}{RT} > 0. \quad (\text{D.1})$$

Isothermal layers are therefore also stably stratified, as is well known. In each such layer, using (10) and the ideal gas law, we find that

$$\nabla_{\mathbf{X}} M(\Theta, \mathbf{X}, t) = \left[\frac{1}{\rho} \nabla p + \nabla(gz) \right]_{\mathbf{x}=\mathbf{X}} = \left[\nabla(RT \ln \eta + gz) \right]_{\mathbf{x}=\mathbf{X}}. \quad (\text{D.2})$$

Hence,

$$M = RT \ln \eta + gz \quad (\text{D.3})$$

up to an arbitrary constant.

Thus, due to (18) again and the continuity of the pressure, at the interface $z = z_\alpha$ between layer α and layer $\alpha + 1$, we find

$$M_\alpha = g z_\alpha + \begin{cases} c_p \theta_\alpha \eta_\alpha^\kappa & \text{if layer } \alpha \text{ is isentropic} \\ RT_\alpha \ln \eta_\alpha & \text{if layer } \alpha \text{ is isothermal} \end{cases} \quad (\text{D.4})$$

and

$$M_{\alpha+1} = g z_\alpha + \begin{cases} c_p \theta_{\alpha+1} \eta_\alpha^\kappa & \text{if layer } \alpha + 1 \text{ isentropic} \\ R T_{\alpha+1} \ln \eta_\alpha & \text{if layer } \alpha + 1 \text{ isothermal.} \end{cases} \quad (\text{D.5})$$

Let N_1 denote the number of isothermal stratospheric layers and $N_2 = N - N_1$ denote the number of isentropic tropospheric layers. Then the analog of expression (23) for the Montgomery potentials reads

$$M_N = c_p \theta_N \eta_N^\kappa + g b, \quad (\text{D.6a})$$

$$M_\alpha = M_N + c_p \sum_{\beta=\alpha}^{N-1} (\theta_\beta - \theta_{\beta+1}) \eta_\beta^\kappa \quad (\text{D.6b})$$

for $\alpha = N_1 + 1, \dots, N - 1$,

$$M_{N_1} = M_{N_1+1} + R T_{N_1} \ln \eta_{N_1} - c_p \theta_{N_1+1} \eta_{N_1}^\kappa, \quad (\text{D.6c})$$

$$M_\alpha = M_{N_1} + R \sum_{\beta=\alpha}^{N_1-1} (T_\beta - T_{\beta+1}) \ln \eta_\beta \quad (\text{D.6d})$$

for $\alpha = 1, \dots, N_1 - 1$. Due to (41), the Hamiltonian satisfying (A.15) and (A.13) is

$$\begin{aligned} \mathcal{H} = & \sum_{\alpha=1}^N \int \sigma_\alpha \left(\frac{1}{2} |\mathbf{v}_\alpha|^2 + g b \right) d\mathbf{x} + \frac{c_p p_r}{g(\kappa+1)} \int \left(\sum_{\alpha=N_1+1}^{N-1} (\theta_\alpha - \theta_{\alpha+1}) \eta_\alpha^{\kappa+1} + \theta_N \eta_N^{\kappa+1} - \theta_{N_1+1} \eta_{N_1}^{\kappa+1} \right) d\mathbf{x} \\ & + \frac{R p_r}{g} \int \left(\sum_{\alpha=1}^{N_1-1} (T_\alpha - T_{\alpha+1}) \eta_\alpha (\ln \eta_\alpha - 1) + T_{N_1} \eta_{N_1} (\ln \eta_{N_1} - 1) \right) d\mathbf{x}. \end{aligned} \quad (\text{D.7})$$

This ends the derivation of the different Montgomery potentials and Hamiltonians relative to the ones for the isentropic N -layer model in the main text.

REFERENCES

- Birner, T., Dörnbrack, A. and Schumann, U., How sharp is the tropopause at midlatitudes? *Geophys. Res. Lett.* 2002, **29**, 10.1029.
- Birner, T., The fine-scale structure of the extratropical tropopause region. *J. Geophys. Res.* 2006, **111**, D04104.
- Bokhove, O., Eulerian variational principles for stratified hydrostatic equations. *J. Atmos. Sci.* 2002, **59**, 1619–1628.
- Bokhove, O., Wave-vortex interactions in the atmosphere, and climate prediction. In *Proc. ICTAM 2004, Warsaw*, eds. W. Gutowski and T.A. Kowaleski, 2005, pp. 103–116.
- Bokhove, O. and Oliver, M., Parcel Eulerian-Lagrangian fluid dynamics for rotating geophysical flows. *Proc. Roy. Soc. A* 2006, **462**, 2563–2573.
- Bokhove, O. and Lynch, P., Air parcel and air particles: Hamiltonian dynamics. *Nieuw Archief voor Wiskunde* 2007, **5**, 100–106.
- Cullen, M. and Feldman, M., Lagrangian solutions of semigeostrophic equations in physical space. *SIAM J. Math. Anal.* 2006, **5**, 1371–1395.
- DiPerna, R.J. and Lions, P.L., Ordinary differential equations, transport theory and Sobolev spaces. *Invent. Math.* 1989, **98**, 511–547.

- Dixon, M. and Reich, S., Symplectic Time-Stepping for Particle Methods. *GAMM Mitteilungen* 2004, **27**, 9–24.
- Frank, J., Gottwald, G. and Reich, S., A Hamiltonian particle-mesh method for the rotating shallow-water equations. In *Lecture Notes in Computational Science and Engineering* **26**, pp. 131–142, 2002 (Berlin, Heidelberg: Springer).
- Frank, J. and Reich, S., Conservation properties of Smoothed Particle Hydrodynamics applied to the shallow water equations. *BIT* 2003, **43**, 40–54.
- Frank, J. and Reich, S., The Hamiltonian Particle-Mesh Method for the spherical shallow water equations. *Atmos. Sci. Lett.* 2004, **5**, 89–95.
- Gill, A.E., *Atmosphere-Ocean Dynamics*, 1982 (New York: Academic Press).
- Holm, D.D., Kupershmidt, B.A. and Levermore, C.D., Canonical maps between Poisson brackets in Eulerian and Lagrangian descriptions of continuum mechanics. *Phys. Lett. A* 1983, **98**, 389–395.
- Li, J. and Wang, S., Some mathematical and numerical issues in geophysical fluid dynamics and climate dynamics. *Commun. Comput. Phys.* 2008, **3**, 759–793.
- Marsden, J.E. and Ratiu, T., *Introduction to mechanics and symmetry*, 1994 (New York: Springer).
- Marsden, J.E., Ratiu, T. and Weinstein, A., Semidirect products and reduction in mechanics. *Trans. Amer. Math. Soc.* 1984, **281**, 147–177.
- Miles, J. and Salmon, R., Weakly dispersive nonlinear gravity waves. *J. Fluid Mech.* 1985, **157**, 519–531.
- Morrison, P.J., Poisson brackets for fluids and plasmas. In *Mathematical Methods in Hydrodynamics and Integrability of Dynamical Systems*, eds. M. Tabor and Y.M. Treve, AIP Conference Proceedings **88**, pp. 13–46, 1982 (New York: AIP).
- Ripa, P., Conservation laws for primitive equations models with inhomogeneous layers. *Geophys. Astrophys. Fluid Dyn.* 1993, **70**, 85–111.
- Salmon, R., Practical use of Hamilton’s principle. *J. Fluid Mech.* 1983, **132**, 431–444.
- Salmon, R., *Lectures on geophysical fluid dynamics*, 1998 (Oxford: Oxford University Press).
- Shepherd, T.G., Symmetries, conservation laws, and Hamiltonian structure in geophysical fluid dynamics. *Adv. Geophys.* 1990 **32**, 287–338.